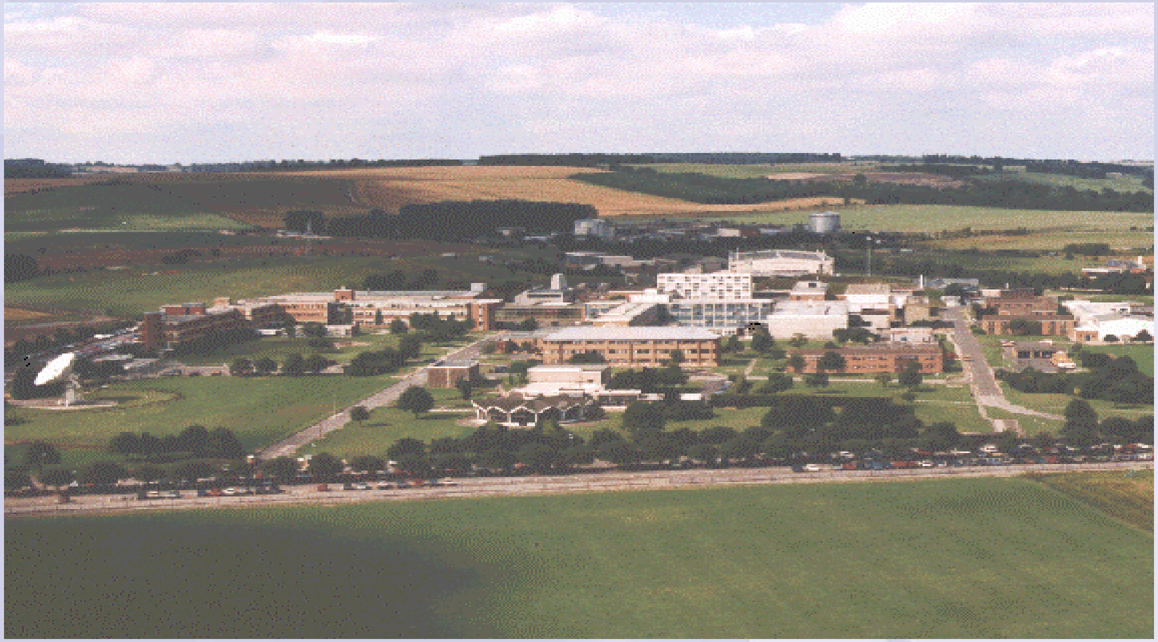
Macromolecular Crystallography and Diamond:

Exciting Prospects with a 3rd generation source

Liz Duke
Diamond Light Source

NSLS-II Workshop
March 15th 2004

From a runway and a green field



To a 3rd generation synchrotron
DIAMOND

Diamond – a little history

- Location: Rutherford Appleton Laboratory, Didcot (south of Oxford)
- Funding:
  - 86% Government
  - 14% The Wellcome Trust
- Cost:
  - £235M for Phase 1
- Phase 1:
  - The machine and 7 beamlines
- Phase 1 Beamlines
  - Beamline 1: Extreme conditions (MPW) (I15)
  - Beamline 6: Materials Science (ex-vacuum undulator) (I16)
  - Beamlines 8, 9, 10: Macromolecular Crystallography (in-vacuum undulator) (I02,I03,I04)
  - Beamline 13: Microfocus X-ray Spectroscopy (in-vacuum undulator) (I18)
  - Beamline 14: Nanostructures Beamline (Apple 2 helical undulator) (I06)

From the SRS to Diamond

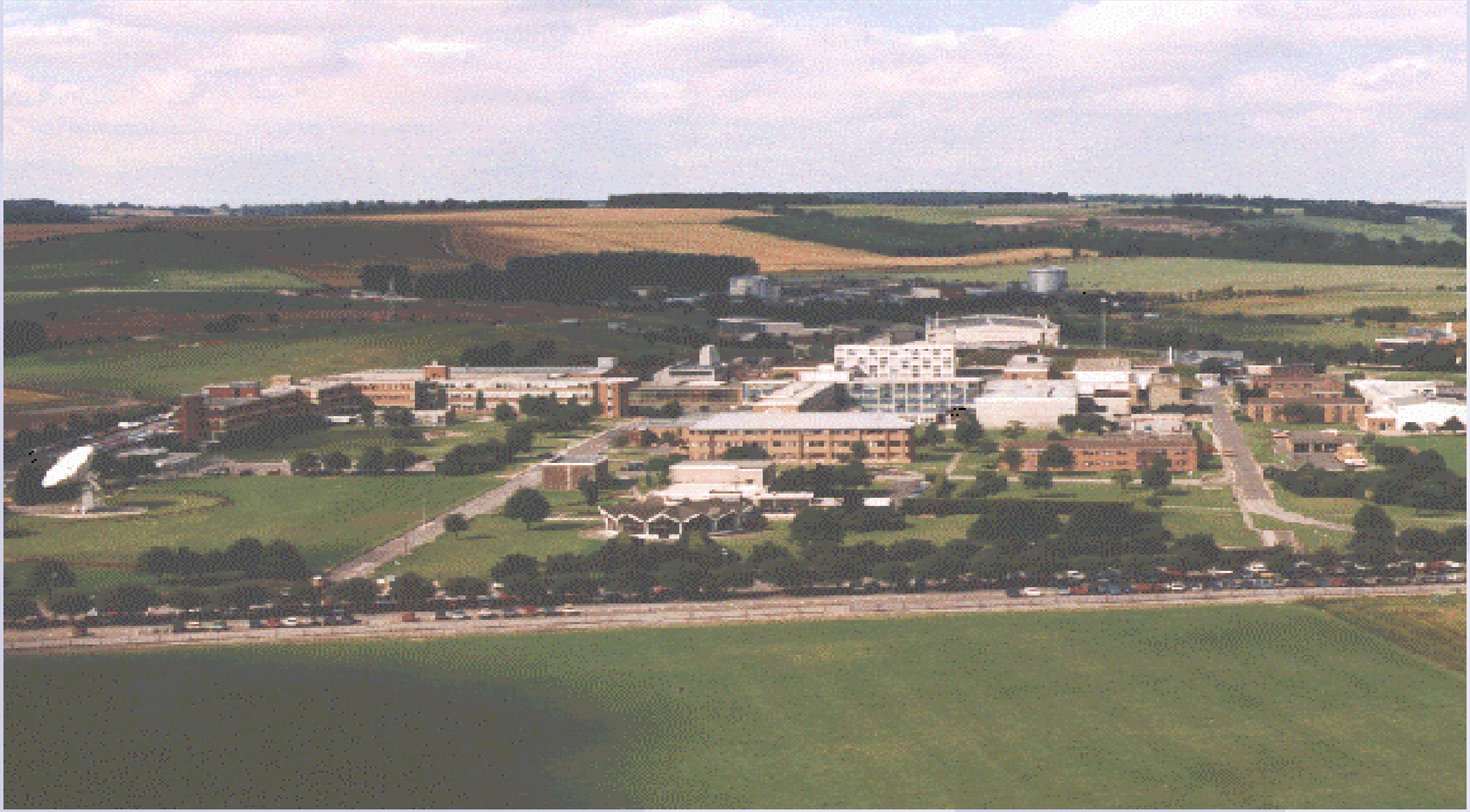
	SRS	Diamond
Energy	2GeV	3GeV
Current	200mA	300mA
Circumference	96m	561m
Number of straights	-	24
Dipole Field	1.2T	1.4T

Diamond Timescales

Formation of Diamond Light Source Ltd	**April 02**
Ground Breaking	**12th Mar 03**
Earliest access to building	**8th Nov 04**
Start of beamline hutch construction	**3rd Jan 05**
Storage ring commissioning with IDs	**7th Aug 06**
Beamlines commissioned with beam	**2nd Jan 07**

diamond

The start

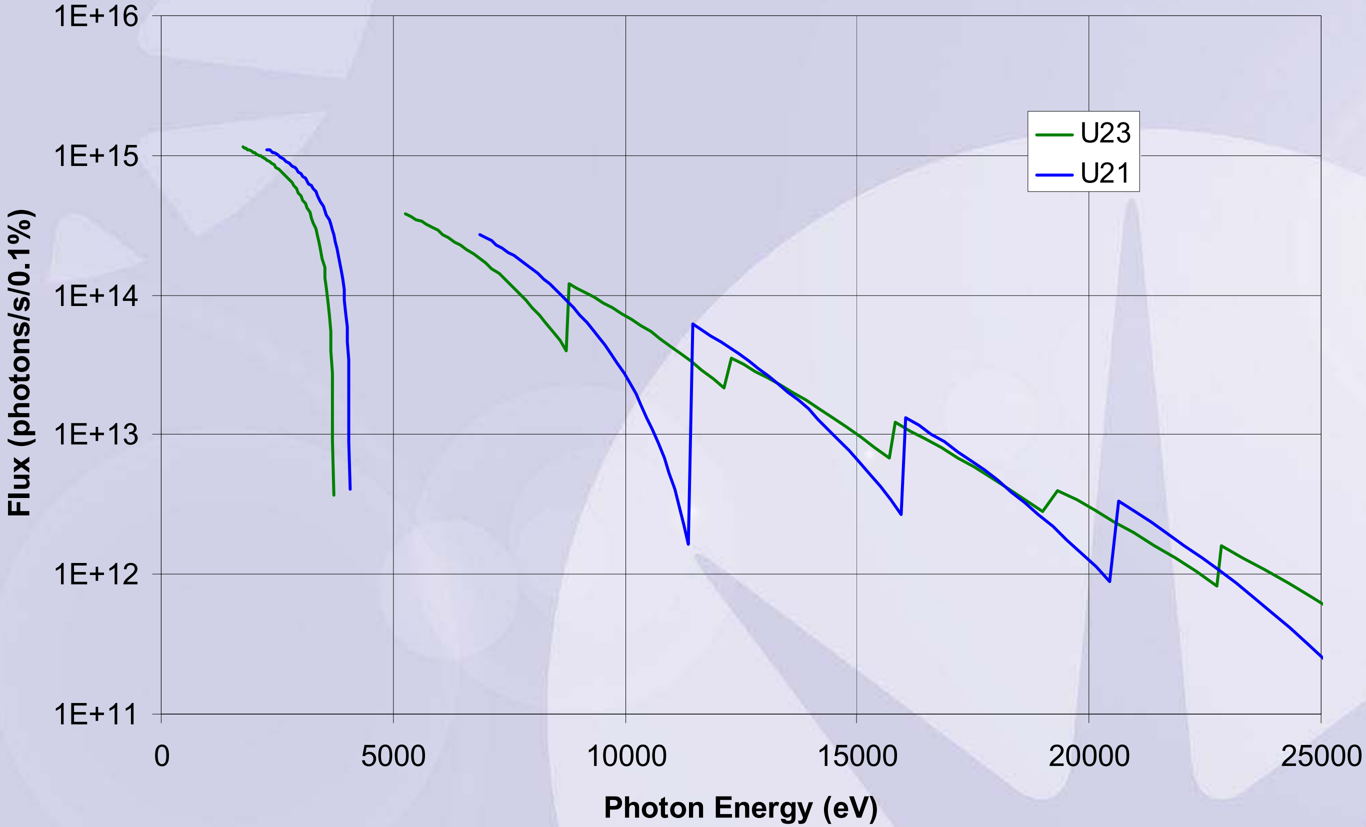


The site 3rd February 2004

Beamline Philosophy

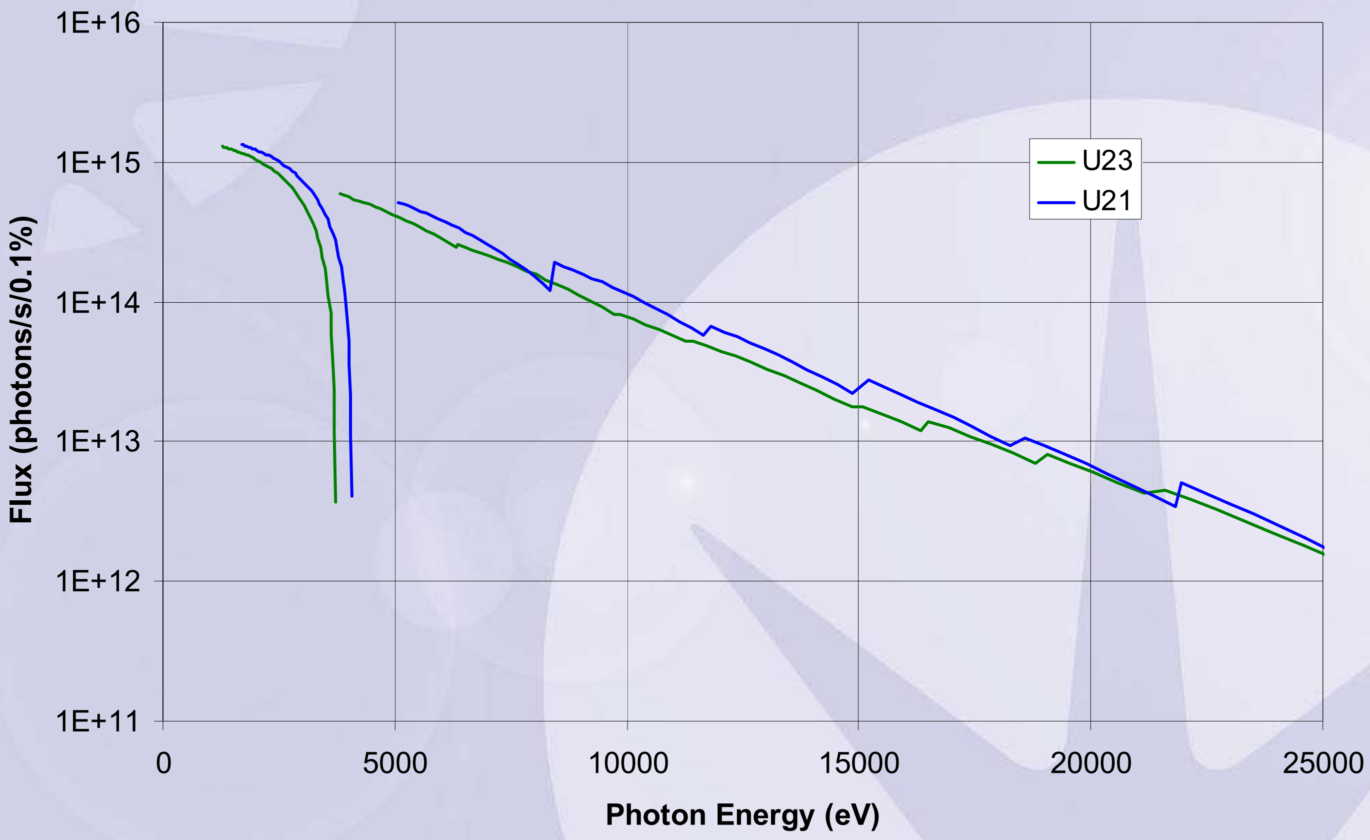
- Designed to enable ease of use for the non-expert whilst catering for the more difficult problems
- All events are seamless to the user
- As automated as possible
  - stability is vital
  - comprehensive diagnostics required
- Requirement for the beamline to be state of the art whilst also ensuring minimal risk

U23 and U21 Undulators at 7mm gap

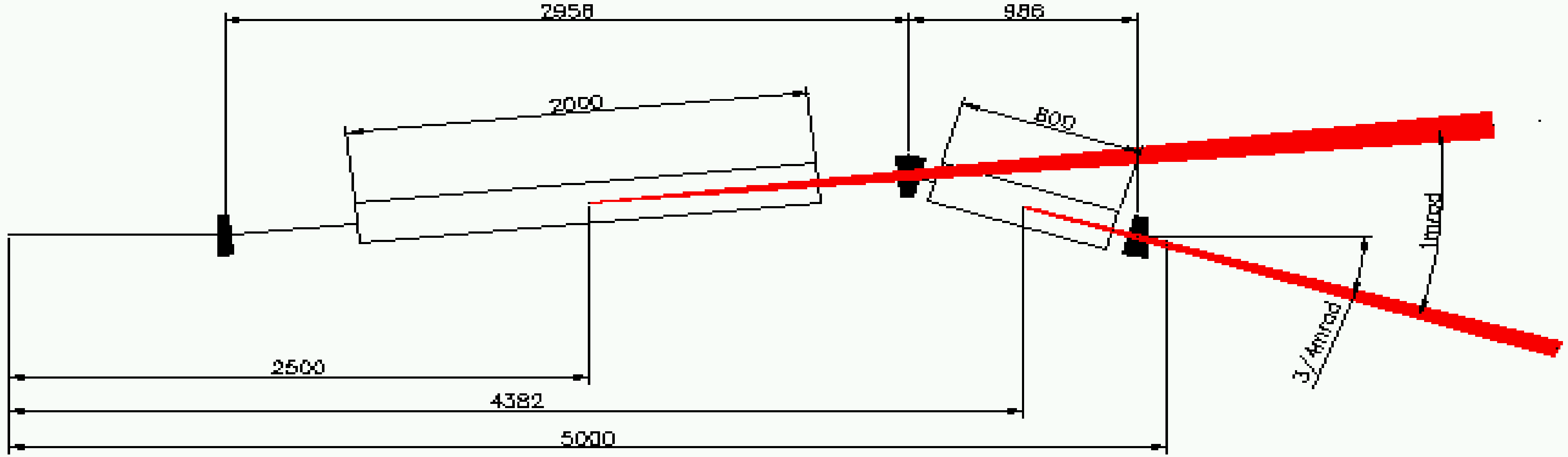


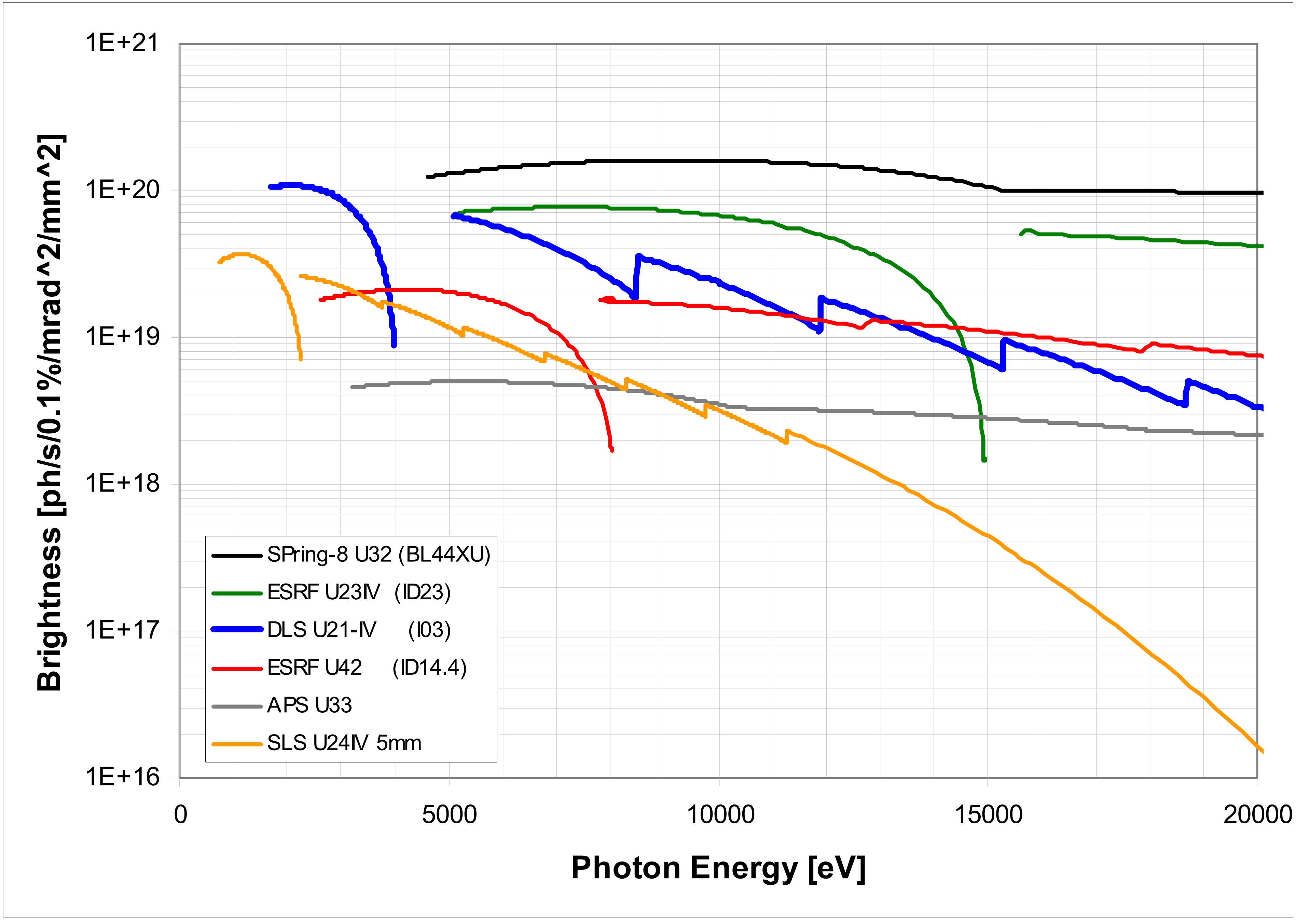
diamond

U23 and U21 Undulators at 5mm gap



Canted Undulators




1E+21
1E+20
1E+19
1E+18
1E+17
1E+16
Brightness [ph/s/0.1%/mrad^2/mm^2]
0
5000
10000
15000
20000
Photon Energy [eV]
SPring-8 U32 (BL44XU)
ESRF U23IV (ID23)
DLS U21-IV (I03)
ESRF U42 (ID14.4)
APS U33
SLS U24IV 5mm

Options for the Optics

	Vertical Focussing	Horizontal Focussing	Wavelength
Option 1	Cylindrical mirror	Sagittal DCM	Sagittal DCM
Option 2	Kirkpatrick – Baez Pair		DCM
Option 3	Torroidal Mirror		DCM

Predicted Overall Focus Size

Options	Focus (h) /µm (sigma)	Focus (v) /µm (sigma)	Focus (h) /µm (FWHM)	Focus (v) /µm (FWHM)	Div (h) /µrad	Div (v) /µrad
DCM + KB Pair	**28.2**	**7.4**	**94**	**17**	**70**	**20**
DCM + Toroid (v)	**24.1**	**15.8**	**87**	**38**	**70**	**20**
DCM + Toroid (h)	**30.9**	**3.2**	**99**	**7**	**75**	**25**
Sagittal DCM + cylindrical mirror	**33.0**	**7.8**	**120**	**20**	**50**	**20**

Assumptions:
Horizontal source size 123µm
Vertical source size 6.4µm
Plane mirror slope errors: 2µrad longitudinal, 4µrad sagittal
Toroidal mirror slope errors: 4µrad longitudinal, 8µrad sagittal
The monochromator makes no contribution to the overall focus

diamond

Optics choice: DCM and KB Pair

- Reasons for choice:

  Ease of use – each component only performs a single task so no coupling
- Fixed exit Si 111 DCM
  - 1st crystal indirectly cooled with LN2
  - 2nd crystal thermally linked to first via braids
- KB mirror pair for focussing
  - Pt, Rh and Si stripes to cover the 0.5Å – 2.5Å wavelength range
  - Planning to use bimorph mirrors – bent electrically via piezos embedded in ceramic which is glued to the back of the mirror

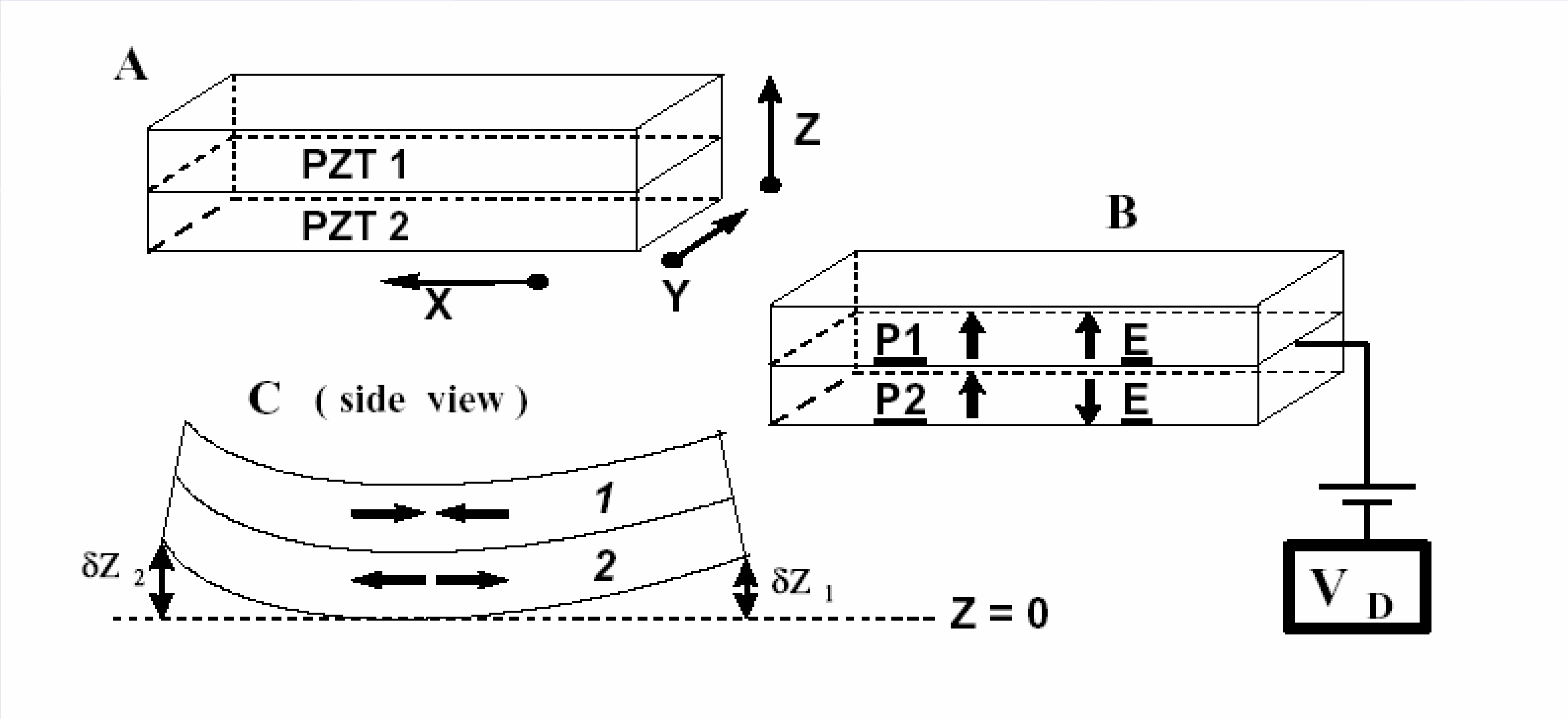
Monochromator Cooling

- Worst case scenario (U21, 5mm gap, 500mA) with monochromator accepting 100µrad x 25µrad at 28m
  - Less than 100W incident on 1st crystal in spot 2.8mm x 2.12mm
- FEA indicates indirect cooling with liquid nitrogen is sufficient to minimise thermal distortions
- Vital to ensure that both crystals are thermally linked

- An alternative being investigated by Soleil is the use of helium (as pioneered here at NSLS!)

diamond

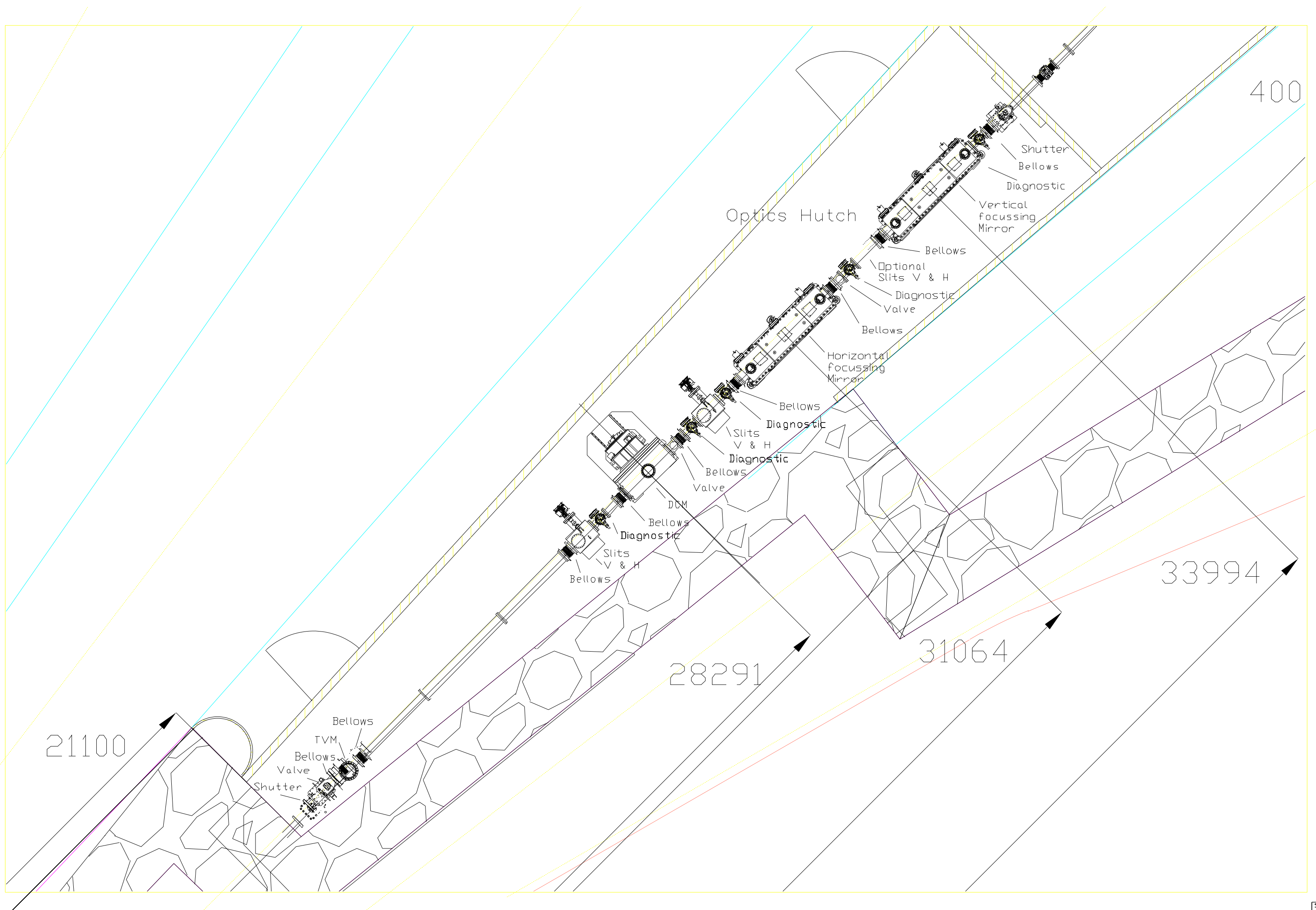
Bimorph Mirrors



Optics Procurement

- Modified turnkey approach
- Economical solution – 3 sets of beamline optics components on 1 contract
- Contract to cover:
  - Mirrors
  - Mono
  - Slits
  - Shutter
  - Diagnostics
  - Controls
  - Vacuum
- Contract has been awarded to Oxford Danfysik

DRG No
A0-
SHT
OF



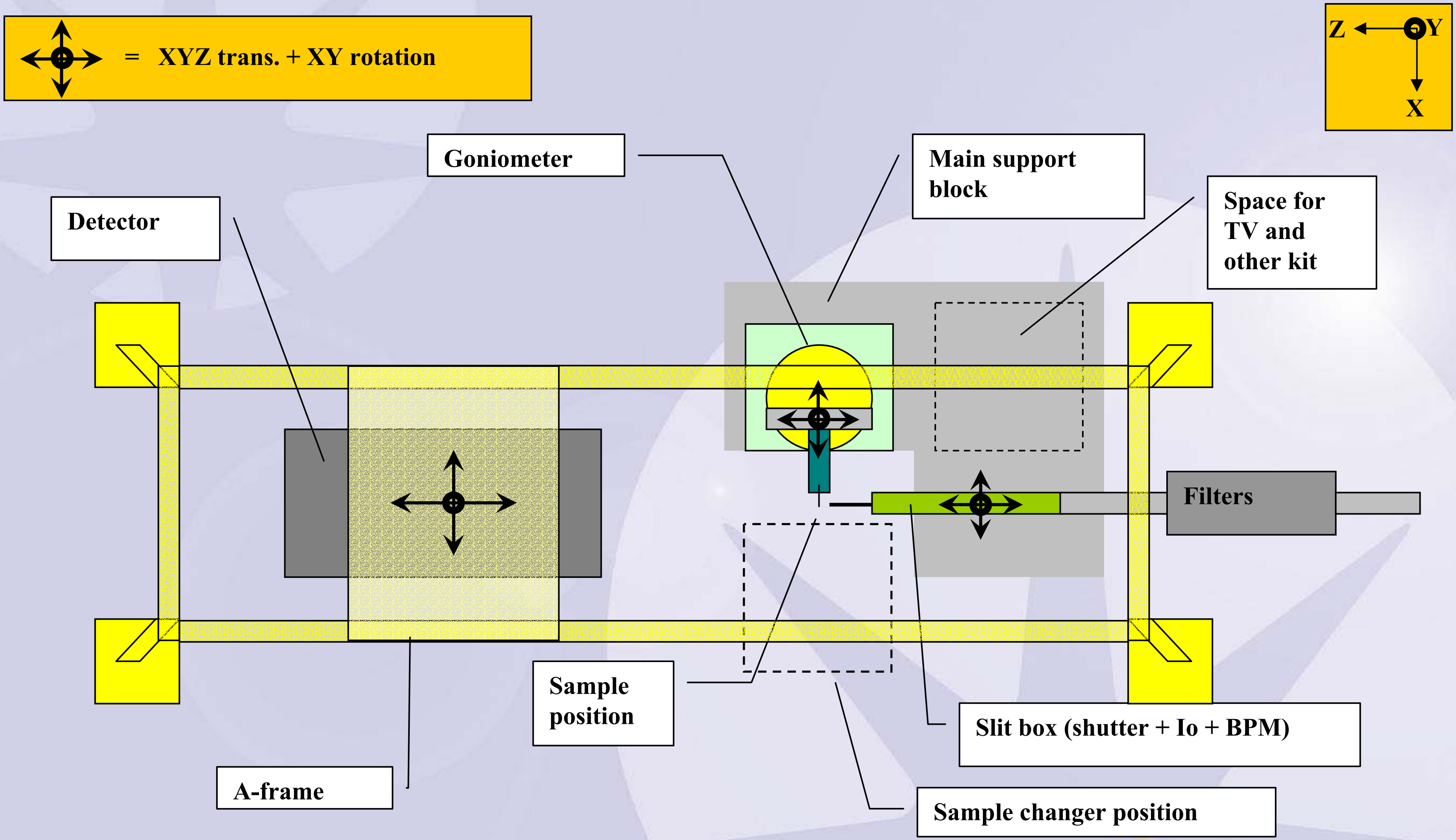
FIRST ISSUE
A

SCALE 0			
ALL DIMENSIONS IN MILLIMETERS UNLESS OTHERWISE STATED			
DRN / DATE	AG / 12/6/03	CENTRAL LABORATORY OF THE RESEARCH COUNCILS DARESBURY LABORATORY CHESHIRE	
CKD / DATE		TITLE PX BEAMLINE 18 (ID2) OPTICS HUTCH 2 LAYOUT PHASE 1 & 2	
CERT / DATE			
APPD / DATE		DRG No A0— SHT OF	ISSUE
		CAD PART No	
DRAWING LIST. –			
CONTRACTORS COMPANY			
CONTRACTORS DRG No			

ORIGINAL FRAME SIZE 1140mm X 790mm

Experimental Station – Issues and Requirements

- MAD
- Designed to deal with very small samples
  - visualisation, stability and reproducibility
- Robotic sample changers
- Automated sample alignment
- Software for automated data collection
- Remote beamline monitoring and data collection
- Category 3 containment on one beamline
- Offline facilities for sample storage and manipulation with basic equipment provided – microscopes, pipettes, facilities for freezing crystals
- Close proximity to research laboratories on the diamond site

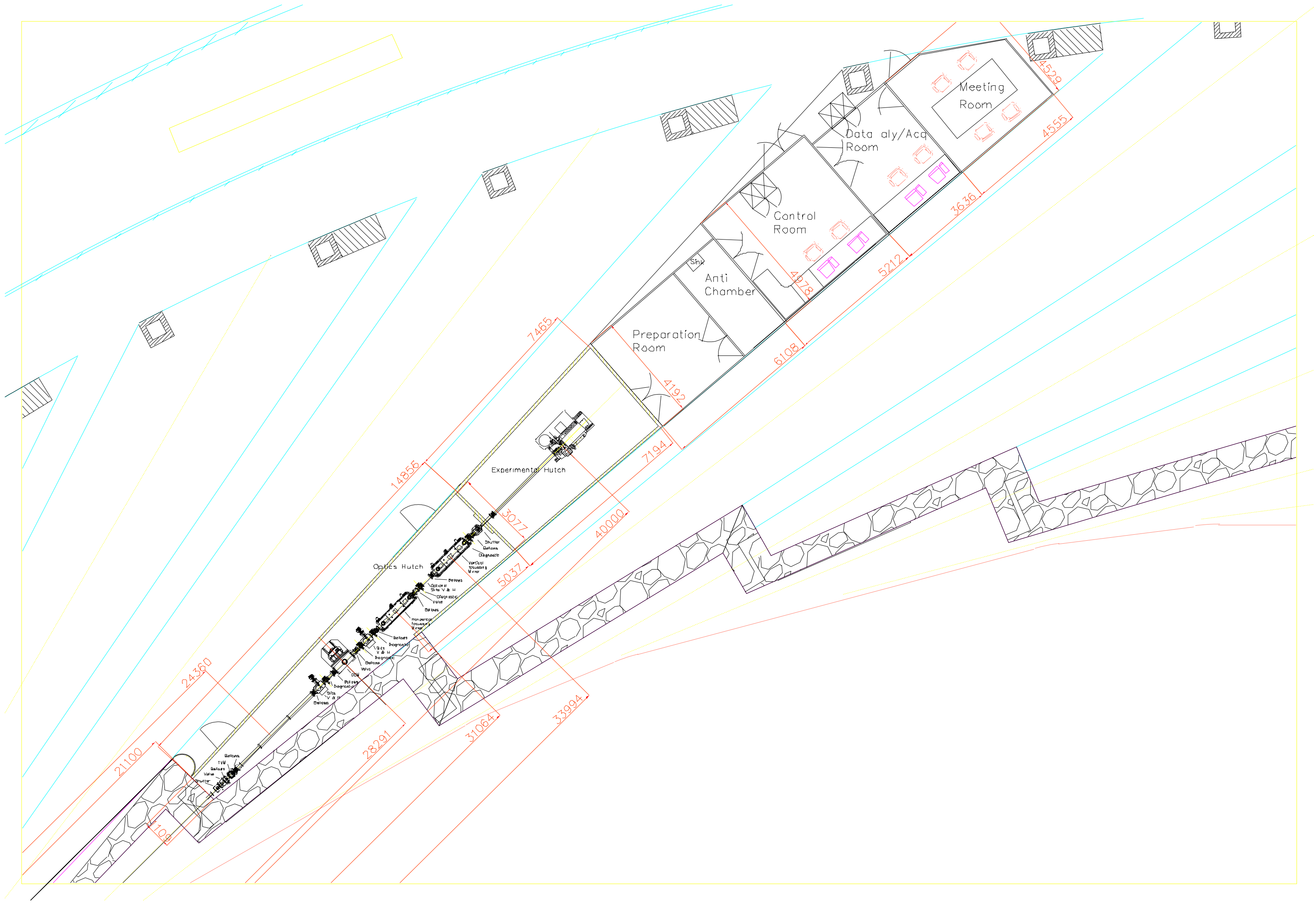


= XYZ trans. + XY rotation
Z
Y
X
Goniometer
Main support block
Detector
Space for TV and other kit
Filters
Sample position
Slit box (shutter + Io + BPM)
A-frame
Sample changer position

Sample Viewing

- Sample viewing from 2 angles – 1 along the axis of the beam
- Fundamental for those who are returning to room temperature data collection on extremely fragile crystals which are grown in the capillary.
- Developed at both ESRF and ALS

DRG No
AD-
SHT
OF



SCALE 0

ALL DIMENSIONS IN MILLIMETERS UNLESS OTHERWISE STATED

DRN	AG	CENTRAL LABORATORY OF THE RESEARCH COUNCILS DARESBURY LABORATORY CHESHIRE
DATE	12/06/03	
CKD		TITLE PROTEIN CRYSTALOGRAPHY DIAMOND BEAMLINE & PHASE 1 ID 2 GENERAL ARRANGEMENT
DATE		
CERT		
DATE		
APPD		DRG No AO— SHT OF ISSUE
DATE		CAD PART No

DRAWING LIST:-

CONTRACTORS COMPANY
CONTRACTORS DRG No

A FIRST ISSUE

ORIGINAL FRAME SIZE 1140mm X 790mm

Biological Containment

- One of the beamlines will have Category 3 level biological containment available at the start.
- The other two beamlines will be designed so as to not exclude an upgrade to Category 3 containment in the future should the need arise.
- Significant requirement of the containment is the requirement to work at negative pressure.
- Requirements for containment will be worked into the automation system and the automation system will be developed to accommodate both frozen and room temperature data collection.

Detectors and Automation

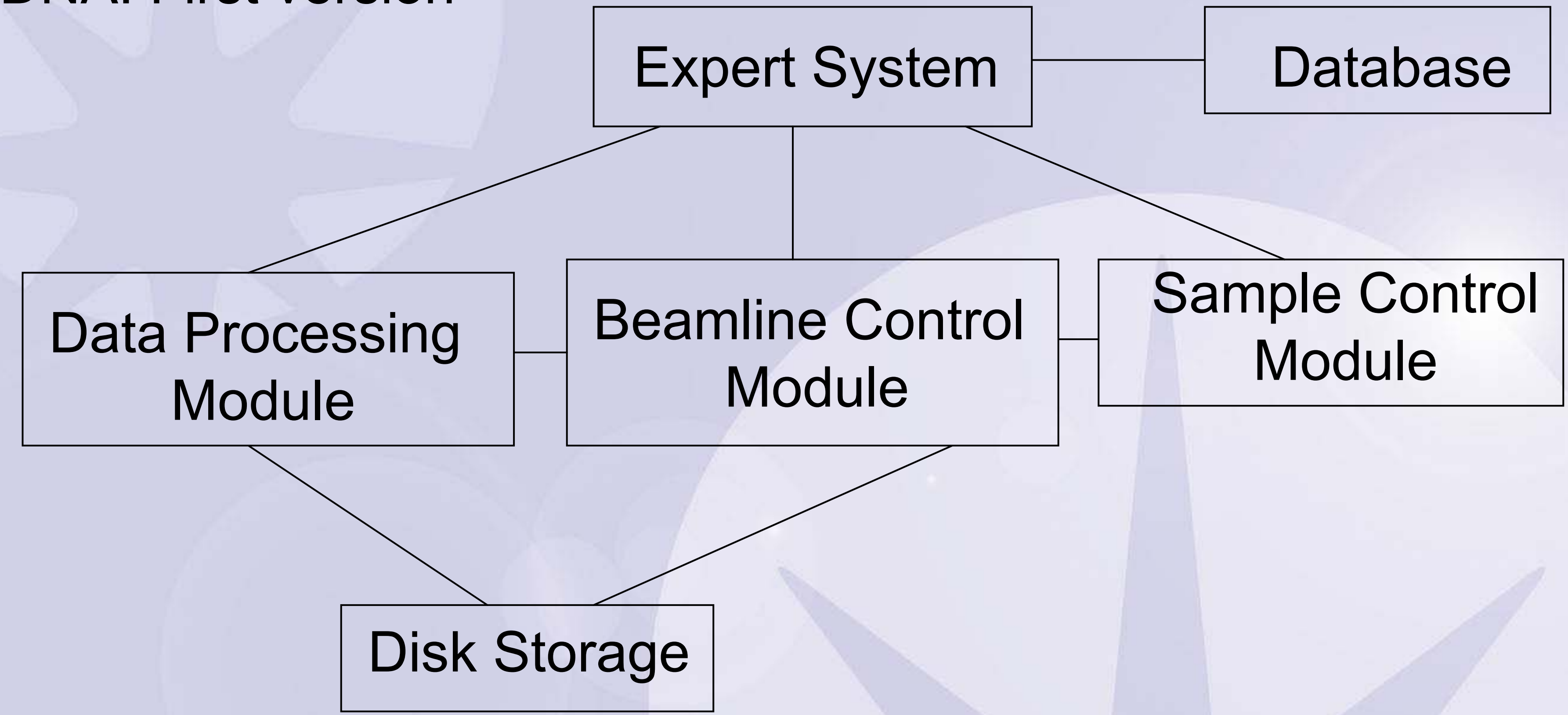
- Commercially procured tiled array CCD detector
- Individual detectors may be different across the beamlines
- All detectors will be procured from the same manufacturer

- All 3 beamlines will be automated on "Day 1" with sample changers
- Aiming to allow remote control of the beamlines and the experiment
- Ultimate aim – the samples arrive unaccompanied, the user controls the experiment from home.

Controls and Software

- Beamline up to end of optics hutch – controls responsibility of controls group in technical division
- Data Acquisition for experiment responsibility of science division
- Machine has adopted the use of EPICS – this will be continued down the beamlines as far as possible
- Requirement for automation implies fundamental requirement for good diagnostics and feedback
- Diagnostics are being installed before and after every optical element
- All motions are to be encoded

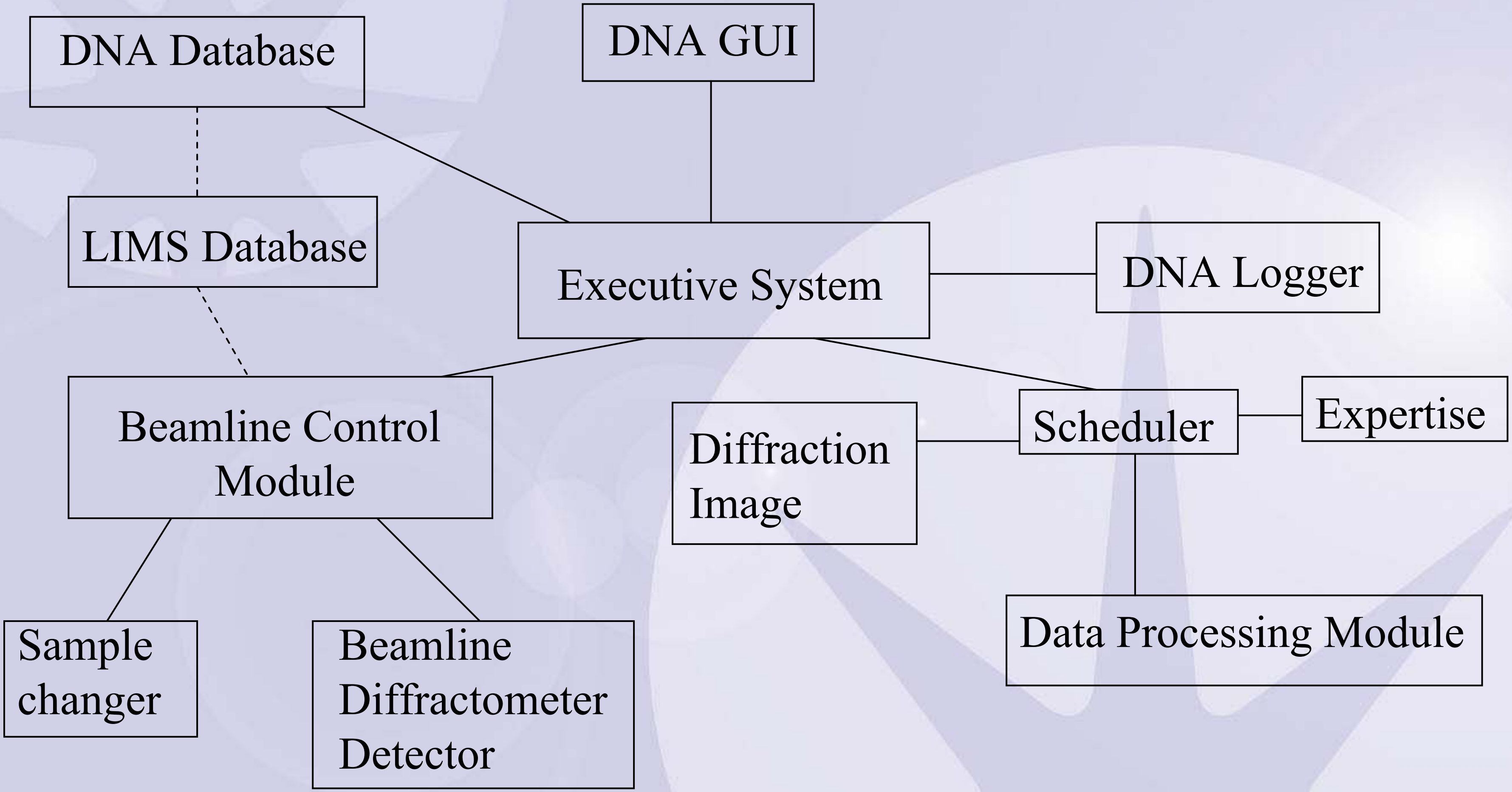
DNA: First version



DNA: Cambridge, SRS, ESRF

“Data nearly automatically”

DNA: Current version



e-HTPX

- **Objectives**
  - to develop a Grid-enabled user interface to allow structural biologists to interact easily with all the required resources for protein crystallography
  - to implement Grid-based portals for protein crystallography, enabling access to all facilities over the internet
  - to implement a Grid-based portal for managing and analysing projects submitted to high-throughput protein production
  - to develop systems for controlling the diffraction data collection and analysis in the context a Grid-enabled resource based on rules as currently used by experts in the field of protein crystallography both at the SRS Daresbury and BM14 at the ESRF. These developments would be made in such a way that they are directly transferable to Diamond, the new UK synchrotron
  - to extend and develop structure determination software to take advantage of low-cost, highly parallel computing facilities (e.g. Linux clusters) so that feedback can be provided on the success, or otherwise, of phasing on the same timescale as data collection
  - to develop a Grid-based application allowing the user to manage flow of data from the initial stages of target selection to the automated deposition of the final refined model in the public databases

Future Beamlines

<u>Approved</u>

- Microfocus beamline (Year 2)
  - Undulator beamline – fully tunable
- Side station
  - Short undulator on 2nd half of cant on one of the Year 1 straights
  - Fixed wavelength (around 1Å)
  - Aimed at projects which don't require *de novo* phase information

<u>Proposal</u>

- Undulator beamline optimised for work at longer wavelengths (up to 2.5Å)

diamond

Comparing Diamond and Soleil

	diamond	soleil
Energy	3GeV	2.75 GeV
Circumference	561.6m	354m
Number of periods	24 DBA; 6-fold symmetry	24 "DBA"
Natural emittance / nmrad	2.7	3.7
Beam size (x, y) / µm	5m: 122.9, 6.4 8m: 178.4, 12.6 Dipole: 53.7, 23.7	3.5m: 388, 8.15
Beam divergence (x',y') / µrad	5m: 24.2, 4.2 8m: 16.5, 2.2 Dipole: 81.4, 2.6	16.3, 8.76
Current	300mA (500mA)	500mA
Straights	18 x 5m 3 x 8m	4 x 12m 12 x 7m 8 x 3.5m

diamond

Comparing diamond and NSLS-II

	diamond	NSLS-II
Energy	3GeV	3 GeV
Circumference	561.6m	550m-600m
Number of periods	24 DBA; 6-fold symmetry	24 TBA
Natural emittance / nmrad	2.7	1.5
Beam size (x, y) / µm	5m: 122.9, 6.4 8m: 178.4, 12.6 Dipole: 53.7, 23.7	54.3, 3.9
Beam divergence (x',y') /µrad	5m: 24.2, 4.2 8m: 16.5, 2.2 Dipole: 81.4, 2.6	27.3, 3.9
Current	300mA (500mA)	500mA
Straights	18 x 5m 3 x 8m	Max 4m

Issues on Diamond –points to note for NSLS-II

- Desire for commonality across beamlines
  - Getting the "standards" right
- Thickness of the lead on optics hutches (30mm Pb) (Gas Bremmstrahlung)
  - Related to the true straight length and vacuum in the straight
- Monochromator cooling
- Good interactions between machine and beamlines
- Diagnostics – electron and photon and feedback between the two
- Continuous status monitoring with parameters stored in a database
- Software and controls